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DTIC FILE COPY Computational Aspects of Adaptive Dimensional Reduction for Nonlinear Boundary Value Problems

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Summary

There has been increased interest recently in feed-back methods for reliable, robust, efficient computational methods in mechanics. We will outline the construction of such methods for a class of problems describing special (anti-plane shear) deformations of bars of rectangular or arched cross section. In particular, we will show how to reduce the dimension of the underlying problem "adaptively". For brittle or linear materials, this method is adaptive (optimal in rate of convergence).

We shall emphasize the computational aspects that have practical import to the performance of this method, such as the construction of a posteriori error estimators that are simple to compute, the selection of basis functions in the dimensional reduction and the heuristic principle for extension. We will illustrate these concepts with computations. *1/10/90*

1. Introduction

Since the dawn of structural mechanics, the scientific and engineering community has pursued the idea of replacing a full system of equations governing the behaviour of "thin" structures by ones posed over their mid surface. We roughly categorize these as follows:

- a physical modelling approach where one uses a priori physical assumptions along with appropriate variational principles to arrive at the dimensionally reduced equations. See [16] for a survey.
- an asymptotic expansion approach. Based on -first- formal asymptotic expansion in a parameter measuring the "thin" dimension, one identifies dimensionally reduced equations - often "justifying" those arrived at above by proving convergence as this "thin" parameter tends to zero - under sometimes very restrictive assumptions. See [4] for a survey.
- an energyasymptotic approach, which is the one we will pursue here. the basic idea is to find a minimizer u_N of the given energy functional in a proper (but still of infinite dimension) subspace V_N which is characterized by some basis functions $\{\psi_j\}_{j=0}^N$:

$$V_N = \{\sum_{j=0}^N c_j(\vec{x}') \psi_j(x_n/d(\vec{x}'))\}$$

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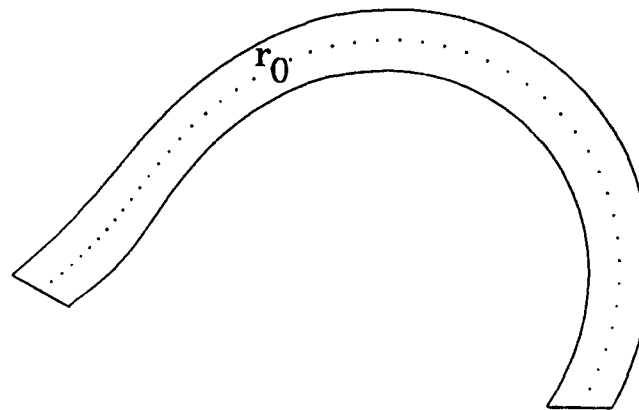
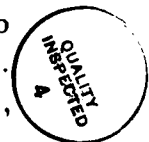


Figure 1: Arch cross section of bar.

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Here we assume that the midsurface is parametrized by the equation $x_n = 0$ and that the thickness of the domain is $d(x^i)$. Thus the model of order N of reduced dimension was introduced. In [6] the choice of $\{\psi_j\}_{j=0}^N$ was made to yield optimal rates of convergence as $d \downarrow 0$ and as by-product also as $N \rightarrow \infty$. This approach goes back at least as far as to Poniatovskii, [15], and Kantorovich, [12].



Undoubtedly, other relevant categorizations may be thought of. If one uses piecewise polynomials for ψ_j and discretizes the Galerkin equations posed over V_N fully by a Galerkin finite element method, again using piecewise polynomials, we may identify the resulting discretization as one of an anisotropic p version using a tensorial basis split along the "thin" direction. We will remain free to choose a full discretization, however. For one dimension there exist robust nonlinear boundary value problem solvers. In addition, the coefficient terms c_j do not coincide with the terms in the formal asymptotic expansion or the reduced solution in the first approach above.

In an earlier paper [6], the method of dimensional reduction for quasilinear boundary value problems was introduced. It was observed that the coefficient functions c_j were concentrated at boundary and interior layers for large j/d . A generalization was proposed which allows for the possibility of different order of dimensionally reduced models in different parts of the underlying domain.

We shall confine our study to the class of problems describing special (anti-plane shear) deformations of bars of rectangular or arched cross section. In fig. 1 we depict an arched cross section with the midsurface being described by the equation - in polar coordinates

$$\Gamma_{\text{mid}} : r = r_0(\theta); \theta \in (0, \omega)$$

The reference configuration for the infinite bar then has a cross section

$$\Omega_d = \{(r, \theta) : r \in r_0(\theta) + (-d(\theta), +d(\theta)); \theta \in (0, \omega)\}$$

We briefly derive the governing equations. During an anti-plane shear a prism with generators parallel to x_3 axis undergo the deformation $(x_1, x_2, x_3) \mapsto (x_1, x_2, x_3 + U(x_1, x_2))$ with a deformation gradient

$$f = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{\partial U}{\partial x_1} & \frac{\partial U}{\partial x_2} & 1 \end{bmatrix}$$

and the left Cauchy-Green strain tensor: $B = ff^T$. For a neo-Hookean, hyperelastic material – i.e. nonlinearly elastic, homogeneous, isotropic and incompressible material – the strain energy is given by $W(\text{trace}B) = W(3 + |\nabla U|^2)$ which in turn determines the Piola-Kirchhoff stress tensor: $S = -pf^{-T} + 2W'(\text{trace}B)f$ up to arbitrary pressure p so that $S_{11} = S_{22} = S_{33} = 2W'(\text{trace}B) - p$, $S_{12} = S_{21} = 0$, and $S_{31} = 2W'(\text{trace}B)\frac{\partial U}{\partial x_1}$, $S_{32} = 2W'(\text{trace}B)\frac{\partial U}{\partial x_2}$. From the equilibrium equations:

$$\sum_{j=1}^3 \frac{\partial}{\partial x_j} (S_{ij}) = 0$$

follows

$$\frac{\partial}{\partial x_1} (2W'(3 + |\nabla U|^2) \frac{\partial U}{\partial x_1}) + \frac{\partial}{\partial x_2} (2W'(3 + |\nabla U|^2) \frac{\partial U}{\partial x_2}) = \text{const.}$$

Identifying $F(|\nabla U|^2)$ with $2W'(3 + |\nabla U|^2)$, the equations are then,

$$\text{div} F(|\nabla U|^2) \nabla U = g$$

with zero displacements prescribed along $\theta = 0$ and $\theta = \omega$ and traction $\beta(\theta)d$ prescribed along $\Gamma_+ = (0, \omega) \times r_0 + d$ and $\Gamma_- = (0, \omega) \times r_0 - d$. F is constitutively given and we take simple power laws:

$$F(t) = 1 + t^n, \text{ for some } n \in \mathbb{N}, \forall t \geq 0 \quad (1.1)$$

Introduce the scaling

$$\rho = \frac{r - r_0(\theta)}{d(\theta)}; \rho \in (-1, 1)$$

Let $u(\rho, \theta) = U(\vec{x})$. Then we relist the equation for the linear case $F = 1$:

$$\begin{aligned} r^2 \Delta U &= \frac{1}{d^2} [(r_0 + d\rho)^2 + (r'_0 + d'\rho)^2] u_{\rho\rho} \\ &+ \left\{ \frac{1}{d} [(r_0 + d\rho) - (r''_0 + d''\rho)] + \frac{1}{d^2} [(r'_0 + d'\rho)d'] \right\} u_{\rho} \\ &- \frac{2}{d} (r'_0 + d'\rho) u_{\rho\theta} + u_{\theta\theta} \\ &= (r_0 + d\rho)^2 f \end{aligned} \quad (1.2)$$

For $n \geq 1$, the algebra becomes more cumbersome but manageable.

Since we use a Galerkin approach we put this into a variational form. Let $\omega = 1$. Find $u \in V$ such that

$$\forall v \in V, \quad Au(v) = G(v) \quad (1.3)$$

where

$$Au(v) = \int_{\Omega} F(|\nabla_a u|^2) \nabla_a u \cdot \nabla_a v \, d\theta \, d\rho \quad (1.4)$$

$$G(v) = d \int_0^1 \beta(\theta) [v(1, \theta)(1 + d) - v(-1, \theta)(1 - d)] \, d\theta \quad (1.5)$$

$$\Omega =]0, 1[\times]-1, 1[\quad (1.6)$$

$$\Gamma_0 = (\{0\} \times]-1, 1[) \cup (\{1\} \times]-1, 1[) \quad (1.7)$$

$$\Gamma_+ = [0, 1] \times \{1\} \quad (1.8)$$

$$\Gamma_- = [0, 1] \times \{-1\} \quad (1.9)$$

$$V = W_{(0)}^{1,2n+2}(\Omega) = \{v \in W^{1,2n+2}(\Omega); v|_{\Gamma_0} = 0\} \quad (1.10)$$

$$\nabla_d = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \left(\frac{1}{d} \frac{\partial}{\partial \rho}, \frac{1}{1 + \rho d} \frac{\partial}{\partial \theta} \right) \quad (1.11)$$

To make the algebra as simple as possible, we worked with the monomials ρ^j as basis in $L^2(-1, 1)$.

This problem corresponds not only to finding a minimizer in V for the energy in anti-plane shear in finite elasticity, [9] and [10] but also to the torsion problem for a bar, see [11] and [13]; then U denotes the Prandtl stress function. See [6]. It is also obtained from Maxwell's equations for the magnetic vector potential related to the magnetic flux density \vec{B} when the magnetic permeability depends on $|\vec{B}|^2$.

2. Dimensional Reduction

We define the dimensionally reduced solution of order N to be the solution u_N in $V_N \subset V$ for which

$$\forall v \in V_N \subset V, \quad Au_N(v) = G(v) \quad (2.1)$$

given V_N a subspace in V of the form

$$V_N = \{v \in V : v(\theta, \rho) = \sum_{j=0}^N c_j(\theta) \psi_j(\rho)\} \quad (2.2)$$

The family of subspaces $\{V_N\}_{N=0}^\infty$ is characterized by the choice of $\{\psi_j\}_{j=0}^\infty$ called the basis or Ansatz functions.

In [6] these basis functions were selected to yield the optimal rate of convergence of $\|u - u_N\|_{H^1}$ as $d \downarrow 0$. We thus had to select ψ_j to be a polynomial of degree $2j$. For F in (1.1) depending on ρ in a more general way, [6] indicated that the same procedure would yield ψ_j to be a nonpolynomial solution of a second order Sturm Liouville problem. (See also [Remark 3.9][7].)

Let us determine the basis functions. Setting $u = \sum_{j=0}^\infty u^{(j)} d^j$ in the PDE for a circular arch:

$$\frac{1}{d^2} [1 + \rho d]^2 u_{\rho\rho} + \frac{1}{d} [1 + \rho d] u_\rho + u_{\theta\theta} = 0$$

yields a formal asymptotic expansion defined recursively by

$$u_{\rho\rho}^{(i+2)} + \{2\rho u_{\rho\rho}^{(i+1)} + u_\rho^{(i+1)}\} + \{\rho^2 u_{\rho\rho}^{(i)} + \rho u_\rho^{(i)} + u_{\theta\theta}^{(i)}\} = 0$$

with $u^{(k)} = 0$ for $k < 0$; the corresponding BC are $u_\rho^{(i+1)} = \beta \delta_{i,0}$ at $\rho = \pm 1$. Carrying this proces out, one obtains that $u^{(j)}$ can be written as a polynomial in ρ of degree j with coefficients that are functions of θ determined intrinsically in the proces. The solution to the Galerkin equations is determined by the span of the basis functions, which then is the polynomials up to degree N . Using the techniques in [6] it is possible to prove convergence as $d \downarrow 0$. Let \bar{u}_N be the N th partial sum in the formal asymptotic expansion as given above, e.g. Let D_1 be the operator defined by $D_1 u = \frac{d^2 u}{d\theta^2}$ mapping $\text{Dom}(D_1) = W^{2,2n+2}(0, 1) \cap W_0^{1,2n+2} \rightarrow L^{2n+2}(0, 1)$. We get.

Theorem 2.1 *Let $n \in \mathbb{Z}_+$. Let $u, \bar{u}_N \in W^{1,\infty}$ be bounded there independently of d . Let $\beta \in \text{Dom}(D_1^N)$. Then there exists C_N independent of d such that*

$$\|u - u_N\|_{H^1} \leq C_N d^{2N+\frac{1}{2}}$$

Regarding convergence of the formal asymptotic expansion for the linear case, we showed in [7] that it is uniformly convergent if d is sufficiently small and β is sufficiently smooth and compatible – it had to be more than analytic: $\beta^{(2k)}(0) = \beta^{(2k)}(1) = 0$, $\forall k \in \mathbb{N}$ and $\exists M > 0$ such that $\forall i \in \mathbb{N} : \|\beta^{(i)}\|_\infty \leq M^i$ – very restrictive conditions. For the partial sum up to index N to exist, one needs the boundary conditions above for $k \leq N$.

Since, for a given practical problem, we cannot depend on d being sufficiently small to ensure that a given tolerance criterion can be satisfied via Theorems 2.1, we have considered in [6] to increase N . Again, optimal rates in this scenario (d fixed, N increasing) were established in [6]. From the computational experience in [6] and elsewhere, it became clear that it was unnecessary (read: wasteful) to increase N uniformly everywhere in $[0,1]$. Rather, there were clearly defined layers (near the boundary and/or rough spots in the load). We propose to increase N near these layers only as our extension procedure.

Let $\mathbf{I} = (0,1) = \cup_{i=1}^m \mathbf{I}_i$, and $\mathbf{I}_i \cap \mathbf{I}_j = \emptyset, i \neq j \forall i, j \in [1, m]$. Let $\mathcal{N} = (N_i)_{i=1}^m$ be an m -vector of nonnegative integers (N_i = no. of basis functions used in \mathbf{I}_i). Consider

$$V_{\mathcal{N}} = \{v : v(\theta, \rho) = \sum_{j=0}^N v_j(\theta) \psi_j(\rho) \text{ such that} \quad (2.3)$$

$$N = \|\mathcal{N}\|_\infty, \quad v_j(\theta) = 0 \text{ for } \theta \in \cup_{j > N_i} \mathbf{I}_i\}$$

a subspace of V_N . Solving

$$\forall v \in V_{\mathcal{N}} \subseteq V_N, \quad Au_{\mathcal{N}}(v) = G(v) \quad (2.4)$$

for $u \in V_{\mathcal{N}}$ is the generalized dimensionally reduced Galerkin problem.

A key ingredient in the selection of the distribution of orders \mathcal{N} – the local a posteriori estimators which will identify the aforementioned layers – will be developed in the following section.

3. A Posteriori Error Estimators

Define the estimator for $(0,1)$ and order \mathcal{N} as

$$Est(\mathcal{N}) = \left\| \frac{1}{d} \frac{\partial e}{\partial \rho} \right\|_{L_2(\Omega)} \quad (3.1)$$

where $e \in H_{(0)}^1(\Omega)$ is the solution of

$$\forall v \in H_{(0)}^1(\Omega) : \int_{-1}^1 \int_0^1 \frac{1}{d} \frac{\partial e}{\partial \rho} \frac{1}{d} \frac{\partial v}{\partial \rho} d \theta d \rho = G(v) - Au_{\mathcal{N}}(v) \quad (3.2)$$

the right hand side being the residual $(Au - Au_{\mathcal{N}})(v)$. Although e is not well defined, $\frac{\partial e}{\partial \rho}$ and $Est(\mathcal{N})$ are, provided the following solvability condition is satisfied

$$\forall c \in H^1(0,1) : \int_0^1 \beta(\theta) 2c(\theta) d \theta =$$

$$\int_{-1}^1 \int_0^1 F(|\nabla_{\theta} u_{\mathcal{N}}|^2) \frac{\partial u_{\mathcal{N}}}{\partial \theta} c'(\theta) d \theta d \rho \quad (3.3)$$

However, this is satisfied (even for $c \in W_0^{1,2n+2}$) if

$$1 \in \text{span}(\{\psi_j\}_{j=0}^N) \quad (3.4)$$

cf. (2.1) and (2.2). This condition is met for any choice of basis functions with optimal rates, see [6].

Similarly define the local error estimator

$$Est_i(\mathcal{N}) = \left[\int_{-1}^1 \int_{I_i} \left(\frac{1}{d} \frac{\partial e}{\partial \rho} \right)^2 d \, d\theta d\rho \right]^{\frac{1}{2}}, 1 \leq i \leq m \quad (3.5)$$

As in [2] we define upper (lower) error estimator to mean

$$\|u - u_N\|_{H^1} \leq (\geq) Est$$

Theorem 3.1 *Let u and u_N be the exact and dimensionally reduced solutions (see (1.3) and (2.4)). Then Est as defined in (3.1) is an upper estimator, i.e.*

$$\|u - u_N\|_{H^1} \leq Est(\mathcal{N})$$

In the language of [3], Est is a guaranteed U-estimator (G-estimator). Also Est is asymptotically exact in the linear case (and under some restrictions in the nonlinear one), i.e. $Est/\|u - u_N\|_{H^1}$ tends to 1 as d tends to zero for β sufficiently smooth. For the nonlinear case, d not small one gets a bound like $Est(\mathcal{N}) \leq C(d)\|u - u_N\|_{H^1}$.

Other estimators are of course possible. A whole class of estimators can be introduced from this residual based approach as indicated in [21].

The localization of the error estimator Est as defined in (3.5) can be founded on exponential decay of the solution away from "vertical" boundaries and/or rough spots in the load as defined in (1.5). The generalized Galerkin problem (2.4) transforms to a system of O. D. E.s whose solution can be bracketed by solutions to two linear ones. These two obey a "St. Venant principle", i.e. decay exponentially away from a concentrated load. See [8]. In fact, for any two optimal bases – spanning the polynomials up to degree N in our case – the exponential decay rates are the same. For example – when the problem is symmetric in ρ –, if $V_N = \text{span}(\{1, \rho^2\})$, the two first decay rates (eigenvalues) are $\kappa_0^2 = 0$ (corresponding to eigenfunction 1) and $\kappa_1^2 = 15$, the latter approximating well the eigenvalue of the full problem $\lambda_1 = \pi^2$ with respect to exponential decay. In contrast, if one omits 1 as the first basis function (nonoptimal), $\kappa_0^2 = 0 = \kappa_1^2$. For $N > 2$, the approximation of λ_1 can not get any worse. For $N = 3$, we already get $\kappa_1^2 = 9.9412 \approx 9.8696 \doteq \pi^2$.

It is possible for each N to diagonalize the system of O.D.E.s in the linear case and even tabulate in advance. However this is not possible to do uniformly for all N and loses importance for the nonlinear case. Since we consider it important to proceed hierarchically, we instead aim at small bandwidth. We therefore choose the basisfunctions as integrals of Legendre polynomials. If the partial sum in the asymptotic series \bar{u}_N exists ($\beta \in \text{Dom}(D_1^N)$ and sufficiently small) and one chooses as the basis the ones from the asymptotic expansion (special combinations of monomials up to degree j – depending on β), one needs only compute the very last coefficient c_N but it is not practical to require this set of circumstances.

4. Adaptivity and Computational Aspects

We now wish to define our feedback extension procedure which under further restrictions turn out to be adaptive, i.e. optimal with respect to convergence rate as $N \rightarrow \infty$. This is the precise sense of "adaptive" due to Babuška and Rheinboldt [17].

We first introduce the heuristic principle which will guide us to an efficient extension procedure based on the local a posteriori error estimators.

Heuristic 4.1 *Let the error associated with the generalized dimensional reduction be estimated by*

$$(\sum_{i=1}^m Est_i^2(N_i))^{\frac{1}{2}}$$

and the cost (work) be estimated by

$$\sum_{i=1}^m \mathcal{W}(N_i, \mathbf{I}_i)$$

Then we aim at achieving

$$Est_i^2(N_i) - Est_i^2(N_i - 1) \propto \mathcal{W}(N_i, \mathbf{I}_i) - \mathcal{W}(N_i - 1, \mathbf{I}_i)$$

by increasing N_i by a factor $\gamma > 1$ where the error-cost quotient is maximal.

Reasoning: Minimizing the error at fixed cost with respect to N_i , yields via Lagrange's multiplier and a backwards difference approximation the proportionality aimed at in the Heuristic.

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A typical choice for workeestimate is

$$\mathcal{W}(N_i, \mathbf{I}_i) = (\alpha_1 N_i + 1)^{\alpha_2} |\mathbf{I}_i| \quad (4.1)$$

for some choice of positive α_i , $i=1,2$.

An easy computation shows that adding one to the relevant N_i will cost one order of N more than the computation of u_N itself and that if one multiplies by γ , Est can be computed at about the same cost as u_N .

Remark 4.2 *Increasing N_i by factor $\gamma > 1$ where necessary is sufficient to obtain a cost of computing Est at the same order of magnitude or less of computing u_N , however it is not sufficient to increase N_i by adding 1.*

Introduce the convergence rate function Φ for any given positive integer N :

$$\Phi(N) = \inf_{\|N\|_{\infty}=N} \inf_{v \in V_N} \|u - v\|_{H^1}$$

We can now state the following theorem about adaptivity w.r.t. convergence rate:

Theorem 4.3 *Let u and u_N be the exact and dimensionally reduced solutions and have gradients bounded uniformly in d . Let $u \in \hat{W}_{(\theta, \rho)}^{(1,r)^2}$ Then*

$$\|u - u_N\| \leq C \Phi(N)$$

The anisotropic Sobolev space $\hat{W}_{(\theta, \rho)}^{(1,r)^2}$ was introduced in [6] and the superpair indicates up to what order generalized partial derivatives (with respect to the corresponding variable in the subpair) are L_2 integrable.

It is possible to extend this result to the case where $m \rightarrow \infty$ as $N \rightarrow \infty$. We here envision computing $Est(\theta)$, $\forall \theta \in I$ and based on this decide whether a bisection and an increase of N in a half interval is beneficial (this is possible using obvious modifications to Heuristic 4.1).

From an implementational point of view, the nice mathematical properties of Est established in the previous section will not suffice, since finding e as a solution of a second order O.D.E. might be too costly. It is possible to find formulae that can be

used to compute e and Est in practice using that e has to be polynomial in ρ which is orthogonal to V_N in the $\int_{-1}^1 \int_0^1 u_\rho v_\rho d\theta d\rho$ inner product. Let $N = 0$, e.g. Then

$$Est^2(\theta) = \frac{2}{3}\beta^2 d^3$$

Note that we selected the monomials as basis merely to be able to formulate $Au(v)$ easily; a change of basis within the same span requires a linear transformation only in order to modify the formulae for the new choice of basis functions.

We next describe briefly our computational experience with the estimator above for the case of a rectangular cross section and a nonlinearly elastic, brittle material. Results for the linear and nonlinear arch will be reported elsewhere. We complement the experiments in [21], where a constant load was treated in the linear case and the viability of a similar estimator was established even for such noncompatible loads. We solve the Galerkin system of ODE's (recast into first order standard form) using the program NLTPBVP developed at Univ. of Maryland, College Park by V. Majer and I. Babuška, see [14] and [1]. We describe the performance in the case of smooth compatible β and $\mu \leq 0$. The exact solution being unknown, we instead use a sufficiently high number of terms in the asymptotic series. We take $\beta = \lambda\pi^2(1 + 3\lambda^2\pi^2\cos^2\pi x)\sin\pi x$. In this case, the reduced solution is $C_0 = \lambda\sin\pi x$. Taking $N + 1$ terms in the asymptotic expansion for purposes of computing the error for u_N is justifiable, since $\|u - u_N\|_{H^1} = \|u_{asy,N+1} - u_N\|_{H^1}(1 + O(d^2))$. We used SMP, cf. [19] to generate the terms and FORTRAN programs for these.

First, in Table 1 we see the results for varying d in the case $N = 0$: θ , the effectivity index is the ratio between the estimated error and the (approximated) true error measured in H^1 . The estimator is within 20 % for domains twice as thick

$d = 10^{-i/2}$ for $i =$	λ	Relative error	θ
0	.1414	1.273	.8109
1	.1414	.3461	1.0232
2	.1414	6.635E-02	1.0550
3	.1414	1.223E-02	1.0583
4	.1414	2.203E-03	1.0587
5	.1414	3.935E-04	1.0587
6	.1414	7.006E-05	1.0587

Table 1: Effectivity indices for $N = 0$.

as long and within 6% when the domain is roughly as thick as long. Est is not asymptotically exact for this nonlinear problem. This overestimation is but 6%. The results for $N = 1$ yield θ values ranging from about .44 at $d = 1$. to 1.06 at $d = 10^{-2}$ and smaller. The efficiency of Est will deteriorate if one moves in any of the following two directions: 1) towards larger values of β or d and/or 2) towards less smooth, less compatible boundary load β . In the former case, the examples computed so far indicate an acceptable performance for all practical values. In the latter case, the localization effect that we will describe later will be of importance, as then Est will be able to recover as one refines (introduces new subintervals in which we can change the orders of the model separately) near a singularity.

In conclusion, the energyasymptotic method for dimensional reduction lends itself well to adaptivity, not only in the sense that the Galerkin system of ODE's is solved using an adaptive ODE solver but also in the sense that it is possible and desirable to carry varying orders of models in differing parts of the underlying domain. Reliable, computable a posteriori error estimators were constructed. The general approach need not be conceptually confined to the class of problems treated here. Our computations suggest a practical confirmation and viability of many of the features described here of this method.

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